Measuring the Fraction of CO_2 in Air with Fourier Transform Infrared Spectroscopy

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Objectives

To measure the fraction of CO_2 in air

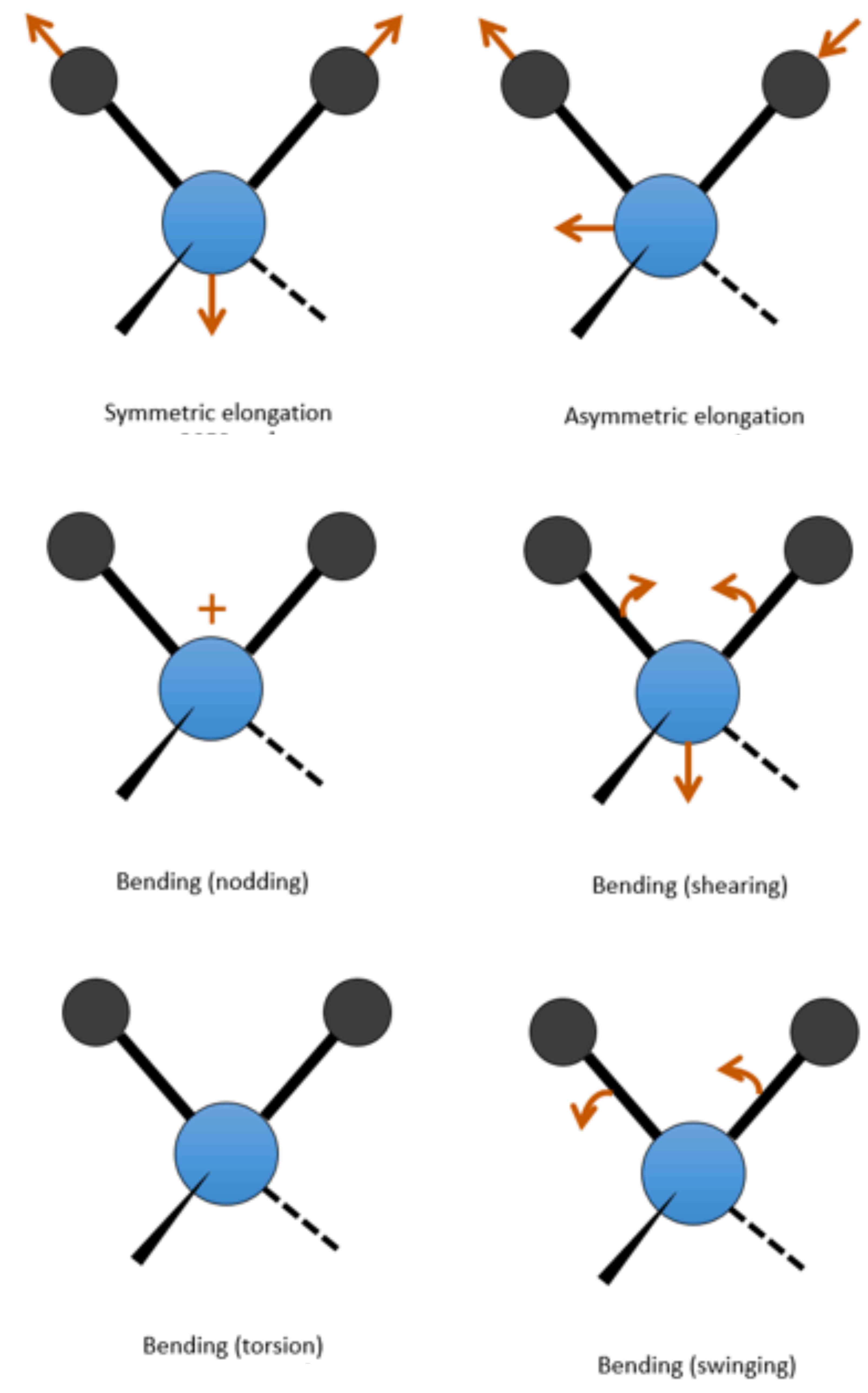
To measure and understand the absorption spectra of N_2, CO_2 and air (aggregation of atmospheric gases)

Theory

In the mid-infrared region of the electromagnetic spectrum, molecules absorb light through the interaction between the photons and the vibrating electric dipoles of the molecule.

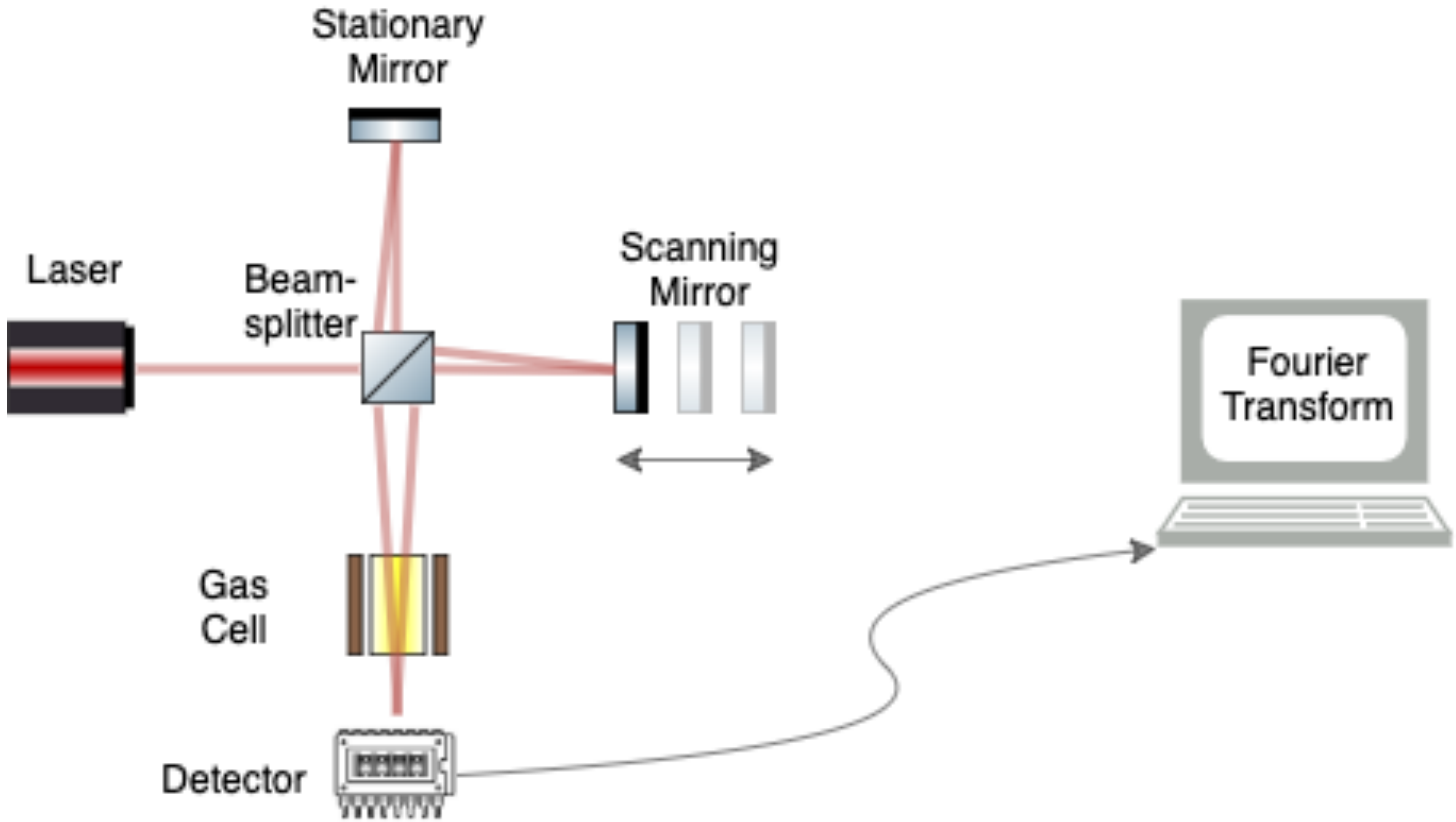
In FTIR, a beam carrying many frequencies irradiates a sample. We measure how much of that beam is absorbed and transmitted by the sample.

With the transmission and absorbance spectra, we can **identify** the molecules in the sample.



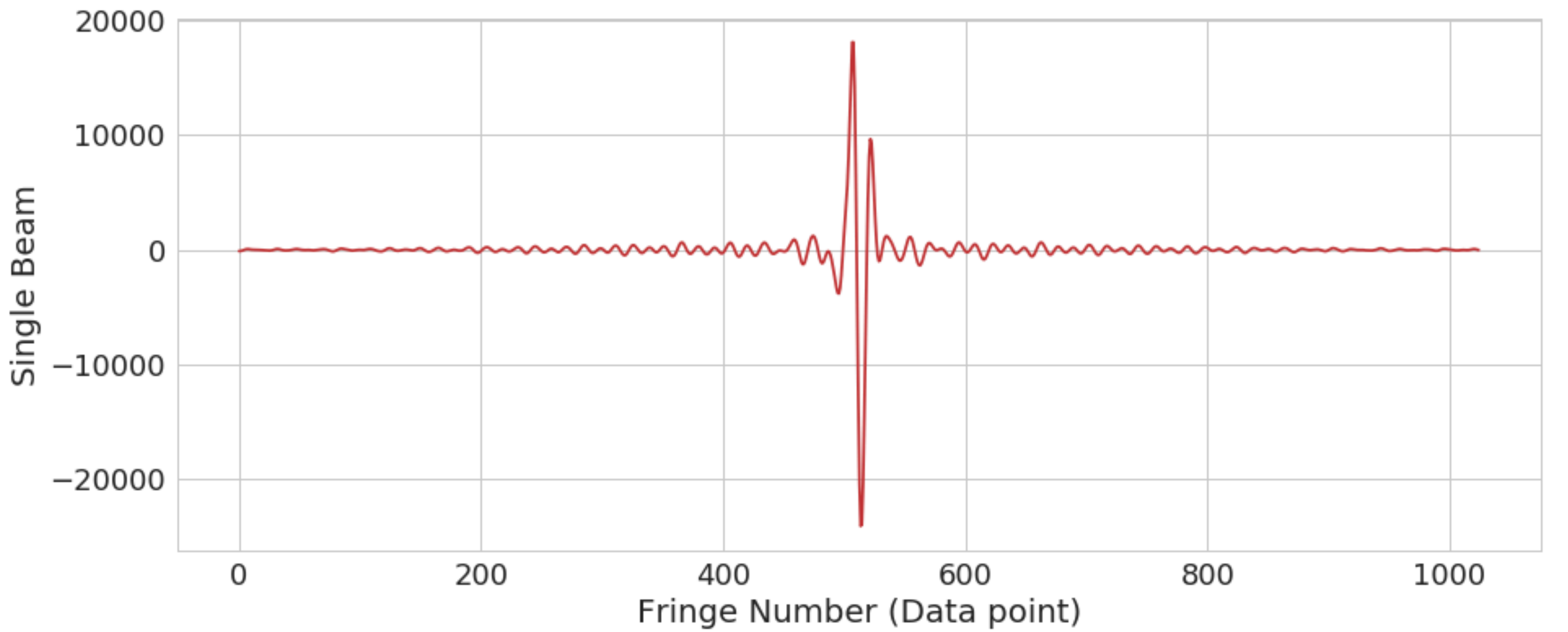
Vibrational modes of molecules
http://brussels-scientific.com/?p=5975

General Setup



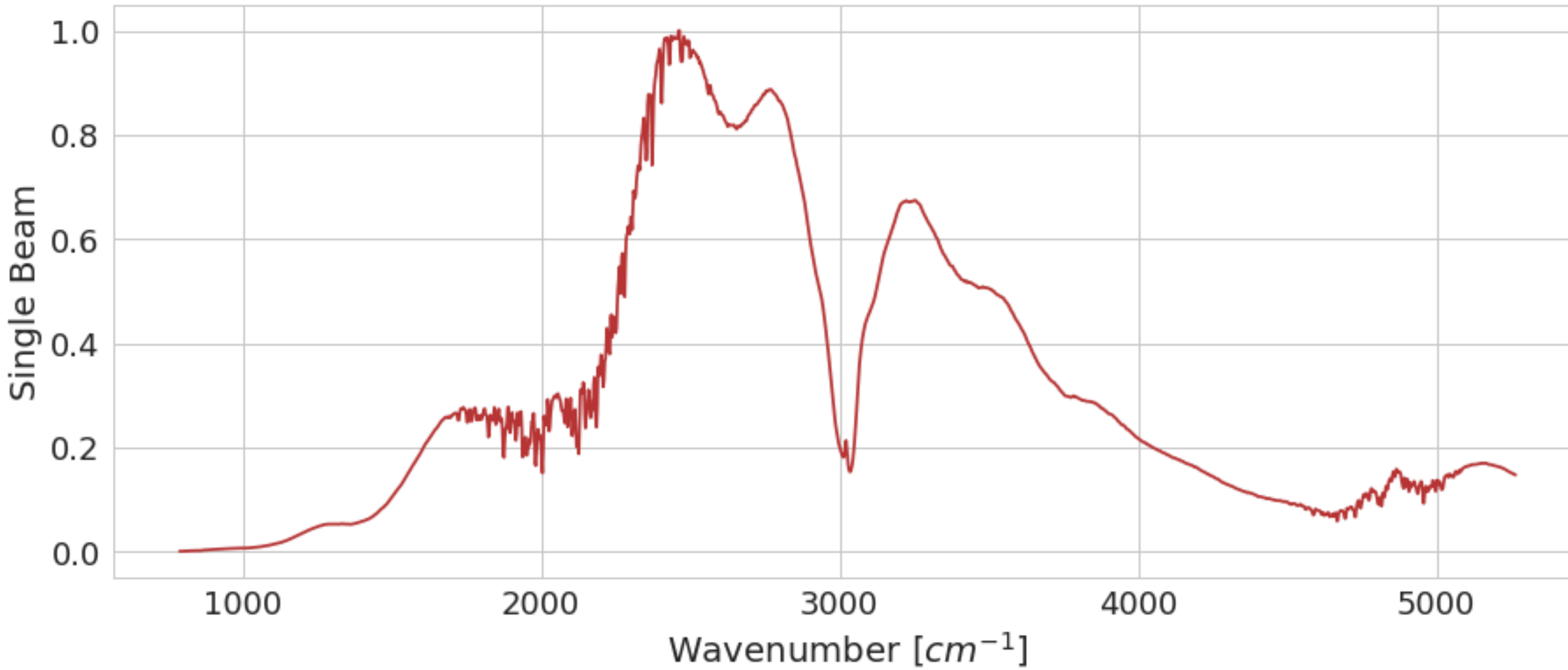
The FTIR is based on the Michelson interferometer. A multimode laser transmits light on the beamsplitter, which splits the light into two beams. The first beam hits the stationary mirror and transmits to the detector through the gas cell. The second beam travels to the scanning mirror. By translating the scanning mirror, different wavelengths in the beam are selected to pass through the gas cell. The detector records the interaction of the beams with the molecules (interferogram) in the gas cell and sends the information to a computer for Fourier Transform analysis.

Method: Data Collection



Interferogram captured with no gas cell, and the FTIR flushed with N_2. We proceed to capture interferograms where the gas cell is in place, flushed with N_2, CO_2, and air, all with FTIR flushed with N_2.

Method: Data Analysis

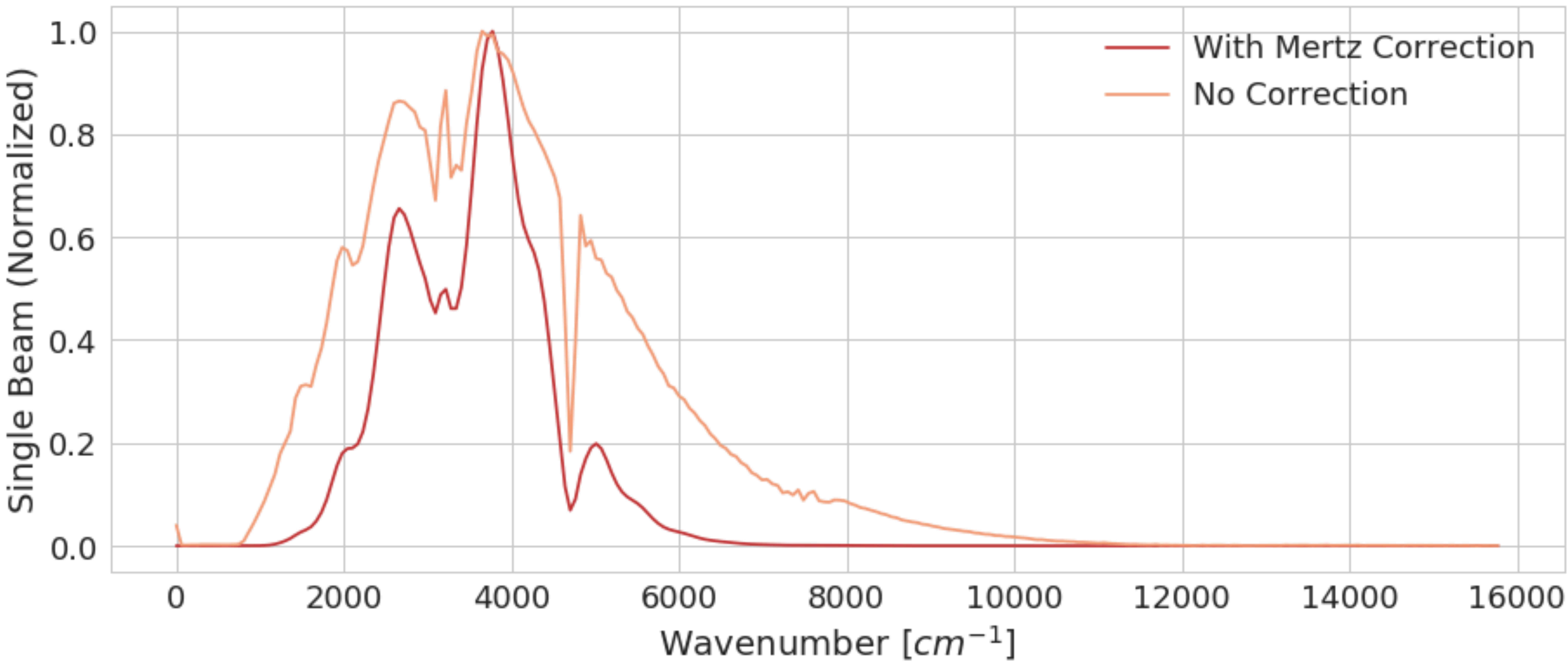


Normalization spectra, collected with a flushed N_2 cell. Mertz correction was applied to smooth noise from from the Fourier Transform. The intensity of this spectra is used to calculate the transmittance and absorbance spectrums for N_2, CO_2 and air with the Beer-Lambert Law:

Transmission: $T = \frac{I}{I_0}$

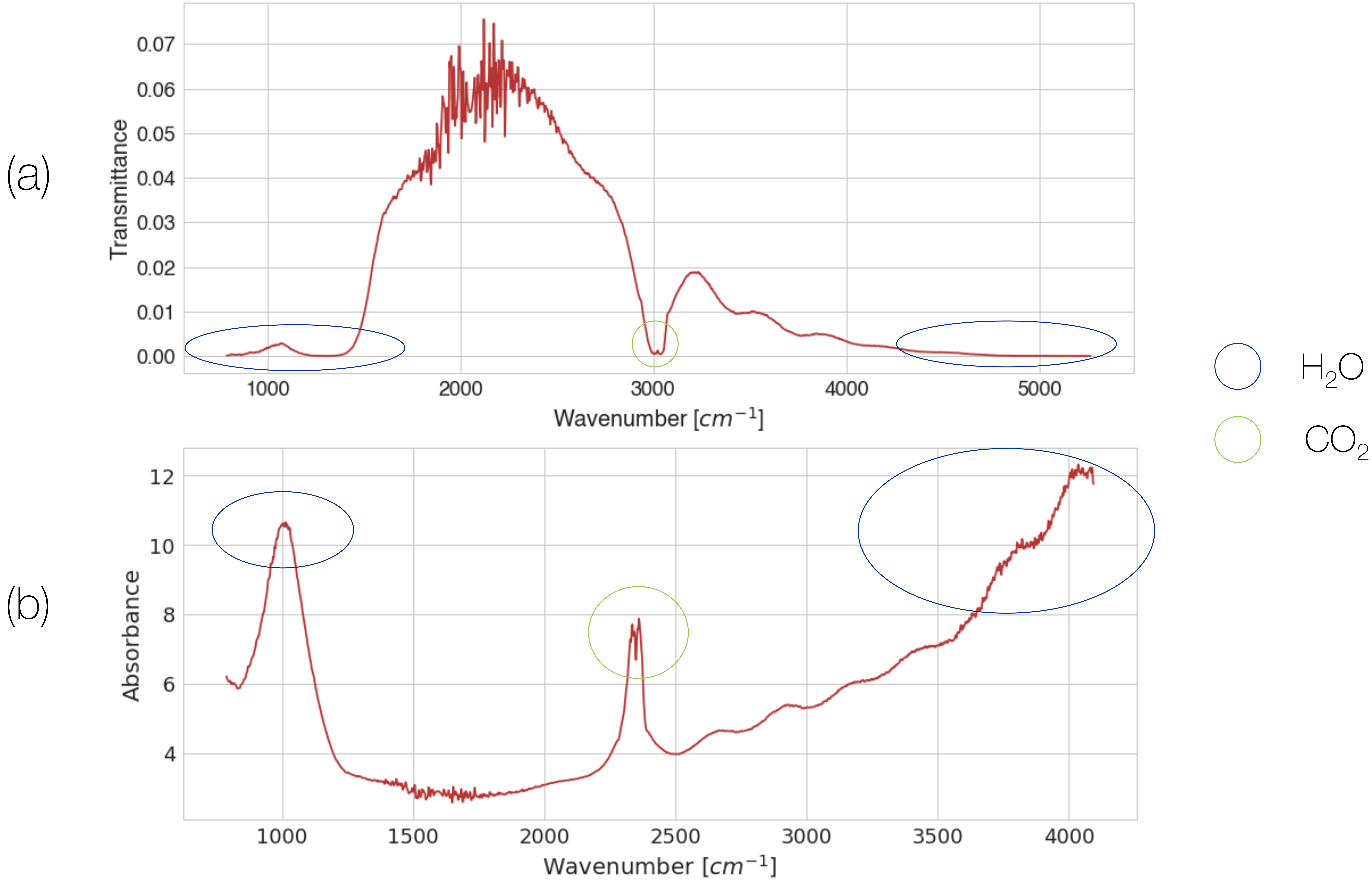
Absorbance: $A = -\log T$

Method: Mertz Correction



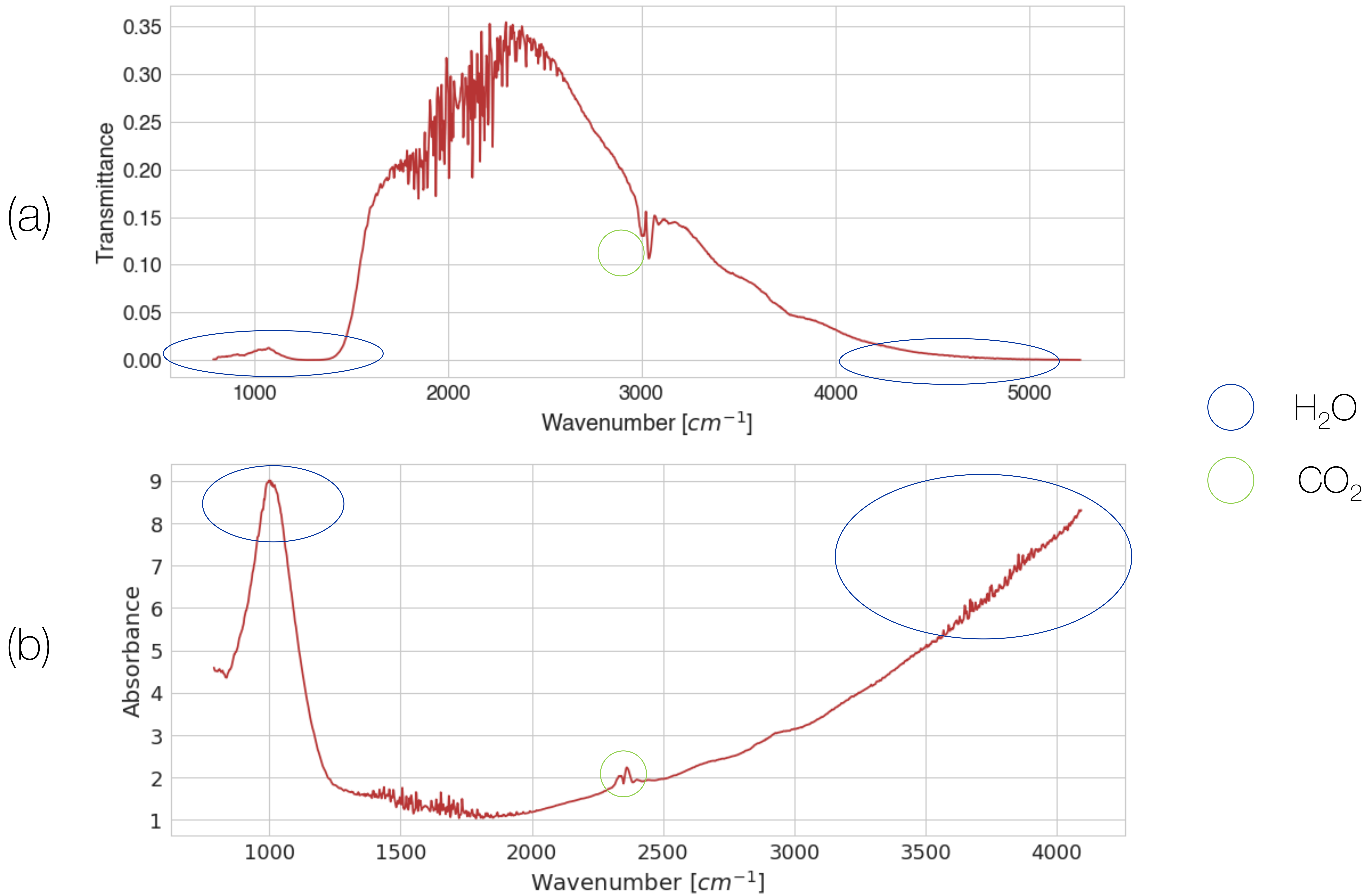
Comparison of spectra with and without Mertz correction. The Mertz correction method modulates the spectra with a triangular signal, to smooth out ringing with taking the Fourier transform of the interferogram. The spectrum with the Mertz correction is smoother and less noisy.

Results: Spectrums of CO_2



(a) Transmission spectra of CO_2. (b) Absorption spectra of CO_2. We see a strong peak around 2350 cm^{-1}, which is where CO_2 absorbs. Hence, the FTIR has identified the CO_2 in our gas cell of CO_2.

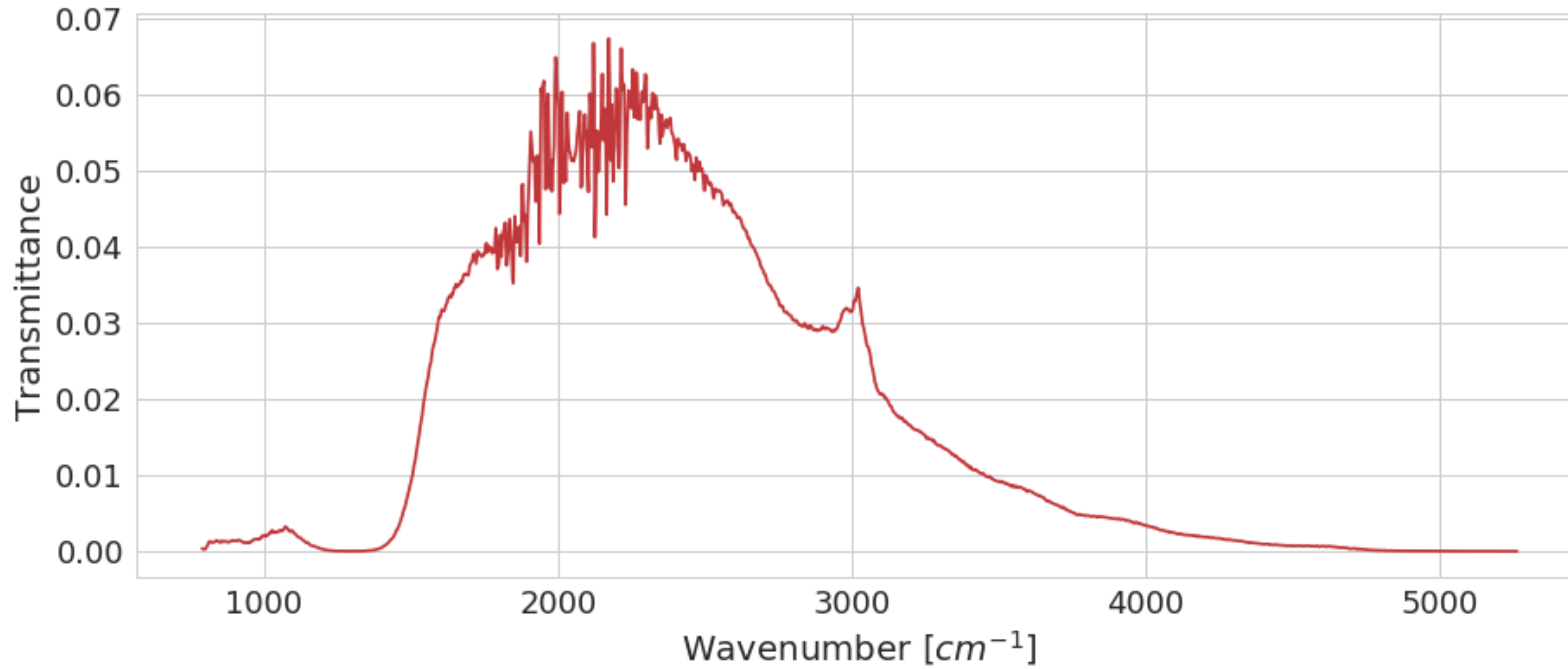
Results: Spectrums of Air



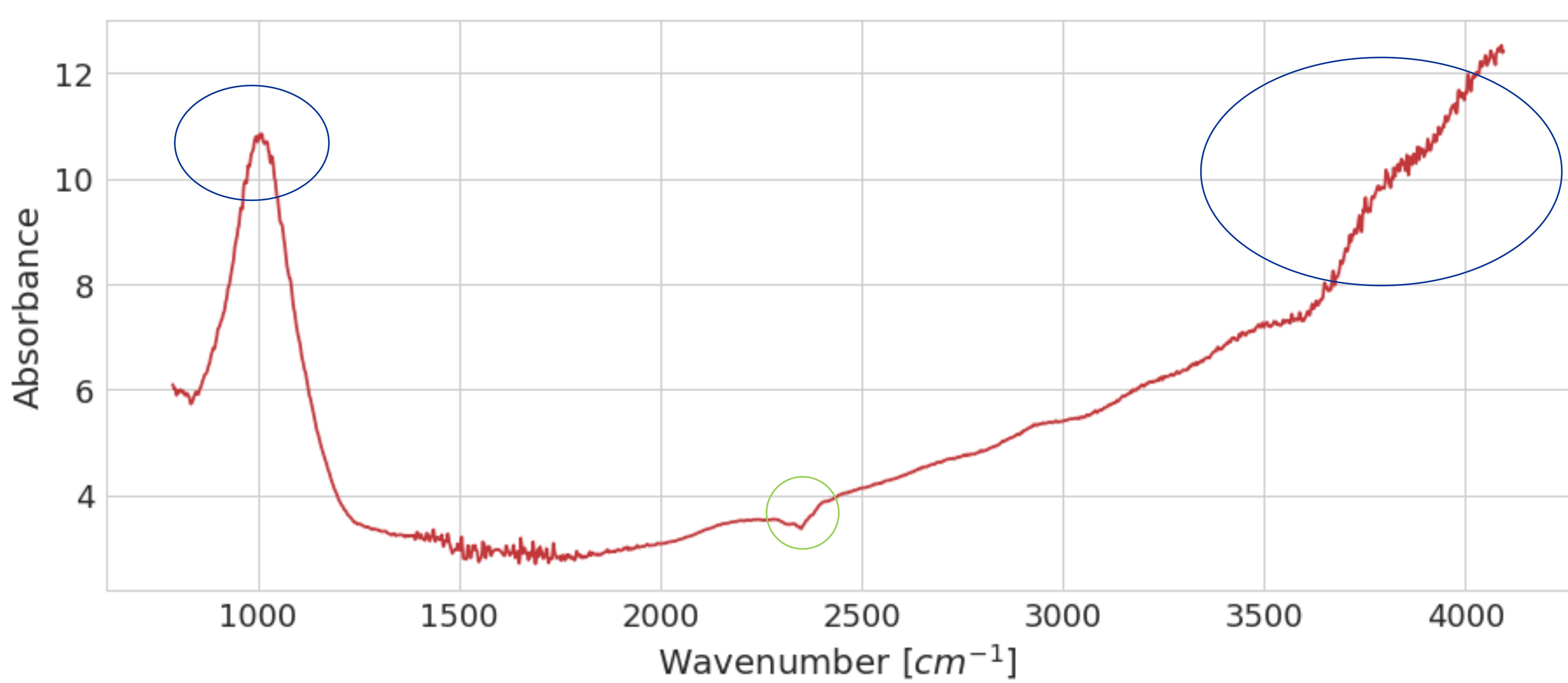
(a) Transmission spectra of air. (b) Absorption spectra of air. We see a weak peak around 2350 cm^{-1}, which is where CO_2 absorbs. Hence, the FTIR has identified the CO_2 in our gas cell of air.

Results: Spectrums of N_2 (control)

(a)



(b)



H_2O

CO_2

(a) Transmission spectra of N_2. (b) Absorption spectra of N_2. We that N_2 does not absorb at 2350 cm^{-1}. This spectrum is very similar to that of air, since air is ~ 75% N_2.

Results: Summary

Molecule	Measured Wavenumber [cm^{-1}]	Expected Wavenumber [cm^{-1}]
CO_2	2352 ± 22	2362

Molecule	Measured Fraction [%]	Expected Fraction [%]
CO_2 in air	8 ± 1	0.04

Conclusions

FTIR is a useful tool for the identification of molecules in gas samples

Lineshape characteristics (width, tail) in FTIR spectrums can be used to infer the type of molecular movements and interactions in the sample

Measurements of gas cells are limited by the thoroughness of flushing